OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Fiscal Year 2004 Transportation Program Highlights

May 2005

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for

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U.S. Department of Energy

OAK RIDGE NATIONAL LABORATORY
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Edmund T. Grostick, Acting Director
W. Keith Kahl, Deputy Director

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Introduction

The Oak Ridge National Laboratory (ORNL) Transportation Program supports the mission of the Department of Energy, Office of Energy Efficiency and Renewable Energy, FreedomCAR and Vehicle Technologies (FCVT) Program through in-house research and development (R&D) activities. Partnerships with industrial companies through cooperative R&D agreements (CRADAs), user agreements, and cost-shared subcontracts are an important part of the program. These partnerships ensure that R&D activities address technical barriers faced by industry in creating components and vehicles that offer increased fuel efficiency that are capable of meeting 2007 and 2010 EPA emissions standards. The Program also addresses longer-term goals of decreasing and eventually eliminating dependency on imported oil in the transportation sector. Projects in power electronics and energy storage are applicable to hybrid and plug-in electric automobiles in the short term, and fuel cell–powered automobiles in the long term. Projects to develop clean diesel engines and diesel exhaust aftertreatment contribute to 21st Century Truck Partnership goals of increased efficiency, reduced emissions, and improved safety and economy in heavy-duty trucks.

ORNL's Transportation Program received approximately $45 million in new budget authority in FY 2004. Partners in industry and academia expended over $12 million in R&D subcontracts, many of them with substantive cost sharing. The Program supported approximately 200 full time–equivalent ORNL technical staff members, and 2 National User Facilities.

Richard E. (Dick) Ziegler, director of the Transportation Program, retired from ORNL in February 2004. We would like to take this opportunity to acknowledge Dick's vision and leadership over the past 12 years. His contributions will be sorely missed.
Edmund T. (Ed) Grostick, Deputy Program Director, was named Acting Program Director as a search for a permanent director was undertaken. W. Keith Kahl was named to take Ed's place as the Deputy Program Director.

This report is organized in two sections. The first section consists of brief summaries of progress during FY 2004 for ORNL R&D projects. The second section consists of detailed descriptions of noteworthy technical highlights and research results.

Project and Program Summaries

Advanced Power Electronics

The Power Electronics and Electric Machinery Research Center (PEEMRC) conducts fundamental research, evaluates hardware, and provides technical support to the FCVT Program, Power Electronics and Electric Machinery activity. In this role, ORNL serves on the FreedomCAR Electrical and Electronics Technical Team, evaluates technical proposals for DOE, and lends its technological expertise to the evaluation of projects and developing technologies. ORNL also executes specific projects for DOE in power electronics, electric machines, and thermal management, in order to help remove technical and cost barriers so that technologies will be suitable for use in advanced vehicles that meet the goals of the FCVT Program.

Significant progress was made in FY 2004 in the development of advanced electric machines and power electronics components for hybrid electric vehicles (HEVs) and fuel cell–powered vehicles. A prototype radial gap interior permanent magnet brushless excitation motor was built by modifying the rotor of an existing off-the-shelf motor. The original motor stator was used in the prototype. This new design with brushless field excitation results in a doubling of the torque at the same full-load current. Additionally, it can widen the speed range and simplify the inverter design.

ORNL researchers developed an integrated dc-dc converter topology that employs only four switches while providing a triple voltage bus (14 V/42 V/high voltage). A 2-kW prototype converter was designed and built. The integrated converter should provide greater reliability, reduced cost, and reduced size, while providing the multiple voltages required by HEVs and fuel cell vehicles.

An integrated traction and compressor drive system employing a five-leg inverter was developed. Researchers designed, fabricated, and successfully tested a prototype inverter with a three-phase induction motor and a two-phase compressor motor. For the compressor drive, the number of inverter components, including semiconductor switches and gate drive circuits, were reduced by more than one-third. The compressor drive was incorporated into the traction motor controller through software, rather than having a separate control circuit, further reducing the cost.

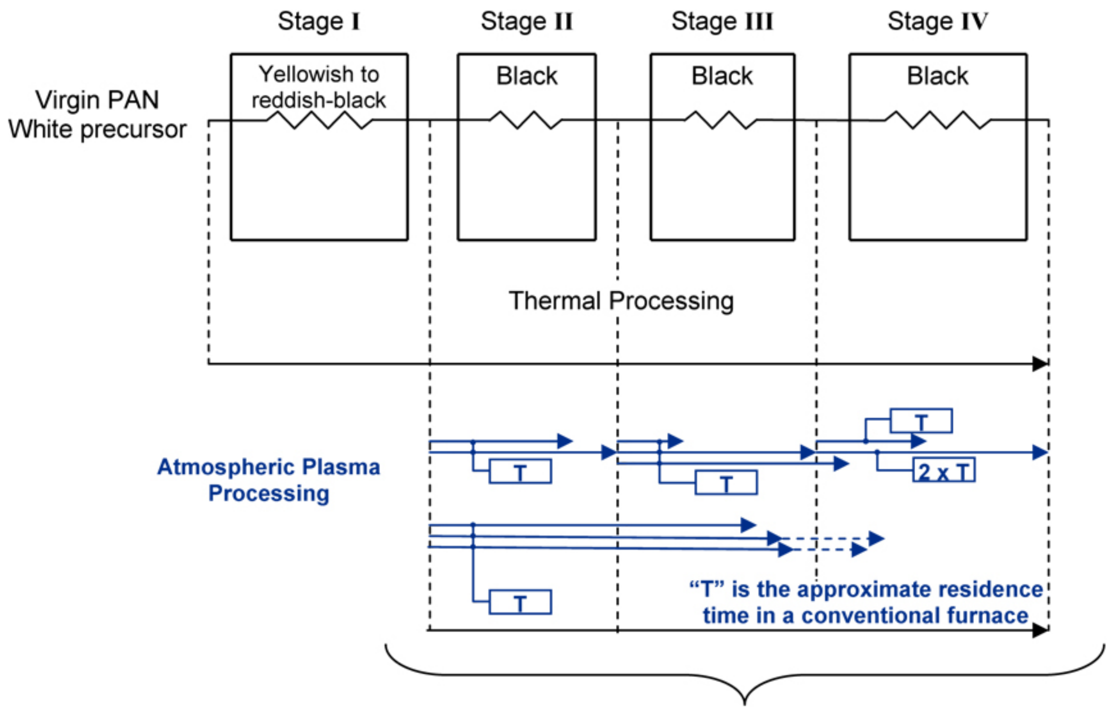
In FY 2004, an extensive analysis of potential motor types was completed to determine their applicability for traction HEV usage. ORNL engineers used a number of analytical models and supplemental calculations to characterize new electric machine designs with the performance characteristics best suited for automotive applications. Physics-based models, recently developed models capable of analyzing new and innovative permanent magnet machine designs, and finite element analysis (FEA) methods were used extensively in the study to evaluate the electric machines.

During FY 2004, ORNL's work on the automotive electric motor drive (AEMD) validation and contract technical support was concluded. ORNL's role for the AEMD project was to provide technical support to DOE, plan and organize the testing phases of the AEMD program, and validate the technology's conformance with the AEMD specification requirements. During FY 2004, the Delphi series electric machine was tested to verify its performance capability.

Automotive Lightweighting Materials

DOE's Automotive Lightweighting Materials Program (ALM) focuses on the development and validation of advanced materials and manufacturing technologies to significantly reduce automotive vehicle body and chassis weight without compromising other attributes such as safety, performance, recyclability, and cost. The specific goals of ALM are to develop material and manufacturing technologies by 2010 that, if implemented in high volume, could cost-effectively reduce the weight of light-duty body and chassis systems by 50% with safety, performance, and recyclability comparable to 2002 vehicles. ALM is pursuing five areas of research: cost reduction, manufacturability, design data and test methodologies, joining, and recycling and repair. Because the single greatest barrier to use lightweight materials is their high cost, priority is given to activities aimed at reducing costs through development of new materials, forming technologies, and manufacturing processes. ORNL conducts R&D activities in all ALM research areas except for recycling and repair. Two areas demonstrating substantive progress in FY 2004 were manufacturing processes for composite materials, and energy management and joining for lightweighting materials.

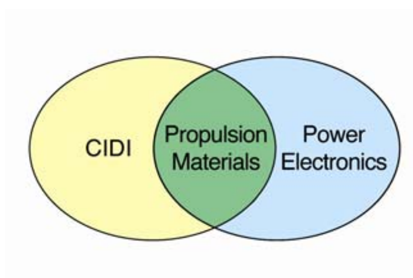
Carbon-fiber-reinforced polymer-matrix composites offer the potential to reduce vehicle weight by 50%. However, cost is a significant barrier to future implementation. Oxidative stabilization of polyacrylonitrile (PAN) precursor is a slow thermal process that typically consumes 70% or more of the processing time in a conventional carbon-fiber conversion line. ORNL is working on a rapid oxidation process that could dramatically increase the conversion line throughput and appreciably lower the fiber cost. They have demonstrated the ability, in atmospheric pressure plasma, to oxidize fiber in stages equivalent to conventional oxidation furnaces; identified key process parameters; modified the reactor to achieve stable operation; and identified the preferred range of feed gas compositions. Preliminary data suggest that the plasma oxidation process may allow earlier onset of carbonization, thus reducing oxidation residence even further. Early economic studies support the value of the research in reducing cost. Continued efforts will focus on continuous plasma processing of multi-tow precursors and characterization of fiber properties.



Schematic of conventional thermal oxidation process and progress in plasma oxidation process.

Two key issues that need to be addressed in ALM are joining and crash energy management. ORNL is working to develop a comprehensive experimental and analytical methodology to analyze and design adhesively bonded automotive composite structures to sustain axial, off-axis, and lateral crash loads. The focus of the project is to develop the understanding of how critical joint design parameters affect the energy absorption. Significant progress has been made in characterizing the static response of bulk adhesive and braided carbon fiber substrates. In addition, preliminary dynamic stability tests on both bonded and unbonded tubes have been completed using the Test Machine for Automotive Crashworthiness (TMAC). The experimental results will be correlated with analytical results by developing finite-element-based tools with appropriate material models and progressive damage algorithms. The results of this project will be closely integrated with the experimental and analytical efforts undertaken by the U.S. Council for Automotive Research (USCAR) Automotive Composites Consortium.

Automotive Propulsion Materials



DOE's Automotive Propulsion Materials Program (APM) engages in R&D that provides enabling materials technology for fuel-efficient and environmentally friendly light-duty vehicles. The APM Program is a partner with the FCVT programs for Power Electronics and Electric Machines, and Combustion and Emissions Control for Advanced Compression Ignition, Direct Injection

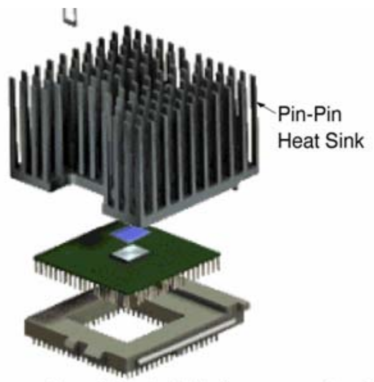
(CIDI) Engines. APM projects address materials concerns that directly impact the critical technical barriers in each of these programs—barriers such as thermal management, emissions reduction, and reduced manufacturing costs. The program engages only the barriers that involve fundamental, high-risk materials issues. FY 2004 featured significant advancements in both materials program areas. In addition, a new project was initiated to develop a low-cost, higher-temperature PEM capable of operating at 120°C without significant degradation due to carbon monoxide (CO) poisoning. This is a collaborative project between ORNL, The University of Tennessee, and The University of Southern Mississippi. If successful, this exploratory project will be transferred to the Office of Hydrogen, Fuel Cells, and Infrastructure or to private industry for future funding and development.

Power electronics. ORNL and Argonne National Laboratory (ANL) are collaborating in the development of higher-strength rare-earth (NdFeB) permanent magnets that will enable significant reductions in the size, weight, and cost of electric motors used in hybrid vehicles. In another project, ORNL is characterizing polymer films, approximately 5 microns thick, which are being developed by Sandia National Laboratories (SNL) as part of an effort to develop smaller, higher-temperature dc bus capacitors. SNL is using the information provided by ORNL to optimize the film properties, in order to minimize manufacturing defects during capacitor winding.

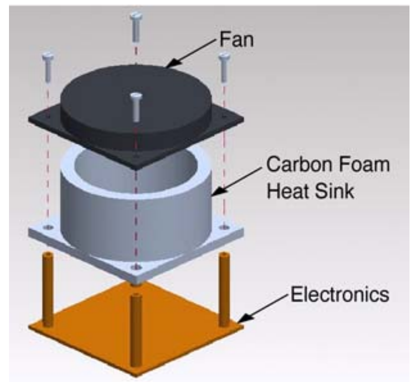
High-power electronic components such as power modules and computer chips being developed for hybrid electric and fuel cell vehicles have ever-growing power requirements. Dissipation of the heat generated by these devices in hybrid electric vehicles often requires an additional cooling loop and water-cooled heat sink to prevent overheating and failure of the devices. The increasing power requirements of electronic devices require that more-sophisticated heat sinks be developed to keep the temperature of the electronics below about 120°C. High thermal–conductivity, high surface–area carbon foam is an innovative new material that offers great potential for advanced heat sinks and heat spreaders.

Porous carbon foam developed at ORNL has an extremely high specific conductivity and an interconnected internal structure that potentially will allow reduction of the thermal resistance of heat transfer devices. Measured cooling rates from a prototype air-water radiator made of carbon foam fins confirm that it can reduce the air-side thermal resistance. During FY 2003/2004, a thermal engineering model to represent heat transfer from porous carbon foam was developed for use in design processes for heat exchangers with finned tubes. Characteristic parameters for carbon foam geometries—exposed surface absolute roughness, exposed surface area factor, effective thermal conductivity, surface-area-to-volume ratio and permeability—are calculated with a simple geometric model of a unit cube with a spherical void surrounded by carbon-foam ligaments. The air-side thermal resistance is calculated with an engineering model derived from conventional correlations that are extended to represent the effects of the rough, porous foam.

During FY 2004, the use of a similar engineering model developed at the University of Western Ontario and tested at ORNL led to the consideration of an alternative design in which all of the cooling air is forced through a thin cylinder of foam. Calculations predict that this simple configuration should dissipate approximately 2× the heat dissipated by conventional heat sinks and aluminum foam devices of similar design. Prototype devices will be built and tested in FY 2005 to verify the designs. Subsequently, it appears that the continued use of models to investigate and develop new carbon foam configurations will be valuable in meeting the increased demand for higher, more efficient heat dissipation.



Conventional heat sink for computer CPU



Alternative configuration for carbon foam CPU heat sink

<u>Advanced combustion engine and emissions R&D.</u> Industrial Ceramic Solutions, LLC (ICS), a small business located in Oak Ridge, Tennessee, is developing a ceramic filter to reduce particulate matter (PM) emissions from diesel engines. Researchers at ICS are working closely with representatives from ORNL, DaimlerChrysler, Ford, and General Motors to develop a filter that will meet the emissions targets of the program. In FY 2004, ORNL conducted scanning electron microscopy on ICS filters (through the High Temperature Materials Laboratory User Program and Technical Assistance Program for Small Business) and identified technical issues that allowed ICS to significantly improve the performance of its filter.

In addition to PM, oxides of nitrogen (NOx) gaseous pollutants in tailpipe emissions are becoming increasingly regulated. Reduction of NOx emissions is an important issue for both CIDI and lean-burn gasoline engines. Several technologies are being developed to reduce NOx emissions, including the lean NOx trap and urea injection systems. Regardless of the method used, accurate and durable NOx sensors will be needed for on-board diagnostics to monitor NOx exhaust levels and for feedback engine control systems to minimize NOx emissions. ORNL, Ford Motor Company, and Lawrence Livermore National Laboratory are collaborating to develop electrochemical solid state NOx sensors based on oxide ceramics. Prototype sensors have shown initially promising sensing characteristics, and ongoing work is being performed to demonstrate the viability of the sensor concept.

High-temperature polymer electrolyte membrane (PEM). Robust, highly conductive, and inexpensive, PEMs allow practical and reliable fuel cell operation at elevated temperatures. The performance of fuel cells is currently limited at temperatures higher than 90°C because of CO and peroxide formation. The use of polymeric membranes able to operate at 120°C would deter CO adsorption, but polymeric membranes are expensive, exhibit limited thermal stability, and are not well suited for high-humidity operation above 100°C. The current benchmark PEM material, Nafion®, is a perfluorinated copolymer with sulfonation to promote water retention and proton conduction, but its conductivity performance drops with increasing temperature and decreasing relative humidity. Furthermore, as a proprietary, fluorated material, it is relatively expensive. The production of hydrocarbon-based polymers for PEM materials is critical to the development of marketable high-performance membranes.

ORNL and University of Tennessee collaborators have synthesized two new classes of materials for potential PEM applications. Poly (phenylene sulfonate) has been synthesized into a thin-film configuration that demonstrates outstanding thermal stability and resistance to inexpensive conventional processing techniques, such as hot-pressing. A fluorinated, sulfonated copolymer of methyl styrene and cyclohexadiene has also been developed that exhibits high thermal stability and improved workability. The application of these materials can prepare the way for energy-efficient fuel cell vehicles by providing thermal and chemical stability under system operating conditions, improved humidity performance through use of functional modifiers, and low-cost processing of non-fluoronated polymers into thin-film configurations.

Thin-film membrane samples of crosslinked, sulfonated poly(phenylene sulfonate) (left) and a fluorinated copolymer of methyl styrene and sulfonated cyclohexadiene (right).

Energy Storage

A new program in advanced battery technology was initiated in FY 2004 by members of ORNL's Condensed Matter Science Division, and Metals and Ceramics Division. Although great progress has been made to improve the lithium-ion (Li-ion) battery technology in recent years, the need for batteries with higher specific power, lower cost, safe and robust performance is particularly acute for the hybrid electric vehicle program. Goals of the new ORNL program are:

- Evaluate the potential for using graphite foam as a high surface current collector for Li-ion and lithium sulfur (Li-S) batteries, and
- Investigate the reaction path and kinetic instabilities at the S cathode and Li anode for Li-S batteries.

The graphite foams developed at ORNL have remarkably high electronic and thermal conductivities which may help alleviate safety concerns of thermal runaway in Li-ion batteries. The pore size, density, surface area, and graphitization of the foams can be widely tailored to optimize the electrode performance. Initial work has characterized the Li insertion reaction with the base graphite material. This is expanding into studies of foams coated with active electrolyte materials.

Current Li-S battery designs are plagued with limited cycle life due to deterioration of the electrode interfaces in the liquid electrolytes, which results in the loss of active battery material. ORNL is investigating incorporation of solid electrolyte layers or protective barriers that may eliminate the deleterious side reactions and electrolyte concentration gradients.

Fuels, Engines, and Emissions Research

ORNL's Fuels, Engines, and Emissions Research Center (FEERC), located at the National Transportation Research Center (NTRC), conducted R&D for multiple FCVT programs in 2004, including Advanced Combustion Engines, Fuels Utilization, and Environmental and Health Impacts. Strong industry collaboration in FEERC is evidenced by 5 CRADAs in engine and emissions technology, plus less formal, yet very active, collaborations with approximately 15 additional private companies and other federal agencies. Some of the CRADAs have resulted in unique research hardware being installed at FEERC. In its role as a DOE User Facility, FEERC conducted a proprietary user project for an important "repeat customer."

FEERC staff are highly engaged in supporting the FreedomCAR and Fuel Partnership and 21st Century Truck Partnership (21CTP) programmatic activities such the Advanced Combustion and Emission Control Tech Team, the Diesel Crosscut Team, and the 21CTP Lab Council. ORNL provides co-leadership, with industry, of the CLEERS activity. In fuels utilization, FEERC staff co-chair three subteams of the Advanced Petroleum Based Fuels-Diesel Emission Control project and sit on the steering committee in partnership with the National Renewable Energy Laboratory (NREL). FEERC staff members also participate on working groups for the Coordinating Research Council. Our facilities and staff are significant participants in the Advanced Reciprocating Engine Systems (ARES) projects in the Distributed Energy Program. Both FCVT and ARES benefit from this leveraging.

There were a number of additions to capabilities at FEERC in FY 2004 in order to stay current with the challenges and research requirements of our partners and DOE. Some of these are listed here:

- Second and third (non-proprietary) full-pass engine electronic control systems were commissioned
- "Gated bagger" for time-resolved emissions speciation
- Further improvements to SpaciMS for in-situ catalyst chemistry measurements

- Fifth engine cell made fully operational that supports two CRADAs, plus a sixth area for small engines
- AVL Indimodule real-time combustion analyzer
- Improved catalyst spectroscopy
- Natural gas engine with lean NOx trap system (ARES)
- Engine models and codes, such as WAVE, have been brought on to aid experiment design and to determine paths to higher engine efficiency
- Electrospray mass spectrometry (for phosphate catalyst poisons from lube oil) and negative chemical ion mass spectrometry (for potentially toxic nitro compounds)
- Methods for "road-side" emissions measurements

Advanced Combustion Engines research is undergoing an orderly shift to more emphasis on improving engine fuel economy through advanced combustion regimes and other technologies, while retaining critical projects on key remaining issues in emission controls. ORNL participates with 14 other organizations in a Memorandum of Understanding on Advanced Engine Combustion Research. Studies are continuing on how advanced combustion regimes might be exploited for inherent efficiency gains in addition to determining the emissions benefits. Powerful capabilities in engine electronic control prototyping were exercised to show quick and near-seamless transition between conventional combustion and low-temperature combustion (LTC). ORNL's approach maintains efficiency while lowering NOx by 90% and PM by about 50%. Research on improving the efficiency of NOx trap regeneration and desulfation was examined by determining which reductants were the most effective. The SpaciMS diagnostic tool was essential in this process. In FY 2004, the SpaciMS was combined with a fiber-optic phosphor-thermometry method for simultaneous chemistry and temperature documentation inside a functioning catalyst. The CLEERS team developed a new standard protocol for characterization of LNT devices. Developed with substantial engine manufacturer input and currently under evaluation, this protocol would enhance current simulation tools for evaluating and optimizing LNT device control architectures. Catalyst suppliers will be able to characterize LNT devices using a single standard sequence of experiments for data distribution to all users. Technical information is posted on a CLEERS website maintained by ORNL. New understanding of urea decomposition processes and products at low exhaust temperatures were developed in an informal partnership with a major catalyst supplier.

In fuels utilization, ORNL participated in completing the studies of how fuel and lubricant constituents such as sulfur and phosphorous can degrade the functionality of emission control devices. Started last year at the suggestion of the Diesel Crosscut Team, development of rapid aging methods for lean NOx traps (LNT) was continued with the aid of a major catalyst supplier. Research on how fuel properties affect advanced combustion regimes [for example, homogenous charge compression ignition (HCCI)] were continued and expanded to include gasoline-like fuels as well as diesel-based fuels. A major energy company is providing test fuels. Initial results confirmed the expectation that new processes such as LTC were impacted by notable shifts in fuel properties. New findings emerged on the effects of fuel properties on LNT functionality. In fact, moderate fuel property variations appear to be not very significant in LNT effectiveness, which is good news for the industry. New reductants, which could be carried by fuel or produced from the fuel on-board a vehicle, were found that gave unprecedented NOx reduction (85-90%) in a passive lean-NOx catalysis system. These data were generated at ORNL in a full-scale engine dynamometer experiment with a catalyst from an industry partner.

In Environmental Science and Health Impacts, FEERC assists in determining the potential adverse impacts of new technologies being developed in FCVT. The Watt Road Environmental Laboratory received funding for real-world truck emissions studies, leveraged by external funding from three new stakeholders: the Federal Highway Administration (FHWA), the Environmental Protection Agency (EPA), and an East Tennessee regional transportation planning organization (sourced from Congestion Mitigation and Air Quality funding). Pending studies will examine ambient air quality impacts from heavy trucks and comparison of the NOx/PM/CO concentrations inside/outside the cabs of idling trucks.

Recently completed work in a PM and aldehyde monitoring study, conducted during winter/summer conditions, revealed significant seasonal differences in fine particulates, with colder weather aggravating the localized ground level PM concentration experienced in the truckstop (from idling trucks). Indeed, regardless of ambient temperature and humidity, PM concentrations were consistently higher in the area of idling trucks (order of 2,500 trucks per day) than those observed at the adjacent major thoroughfare (order of 25,000 trucks per day). Similarly, concentrations of aldehydes were also observed to be above levels warranting health concern.

ORNL hosted the Third Project Review Meeting on the Watt Road Environmental Laboratory Initiative (WRELI) on July 28-29, 2004. Attendees and presenters included representatives from The University of Tennessee (WRELI partner), NREL, West Virginia University, University of Maryland, Virginia Tech and California's Energy Commission (California Air Resources Board). Discussions highlighted the choices and merits of different technologies for remote interrogation of emissions (for example, LIDAR, ultraviolet light absorption, and acoustical). A key technical challenge is to extract useful vehicle emissions information while differentiating it from background emissions sources such as biogenic hydrocarbons.

There were a number of other new projects at FEERC mentioned briefly below:

- Diesel exhaust species data summary (for the Coordinating Research Council)
- Emissions characterization of marine (U.S. Navy) engines was conducted via offsite assistance
- NOx aftertreatment for hydrogen internal combustion engines
- Application of SpaciMS to fuel cell stack, intra-stack hydrogen and oxygen measurements

- Determination of interferences with wide range air:fuel ratio sensors in rich diesel exhaust
- Partnership with University of Tennessee on thermodynamic analysis of HCCI (with the University being funded by the Department of Defense)

Heavy Vehicle Propulsion Materials

Advanced materials are an enabling for fuel efficient heavy-vehicle truck engines. The Heavy Vehicle Propulsion Materials Project is organized around the following technology issues: fuel systems; exhaust aftertreatment; air handling, hot section, and structural components; and standards.

Materials for fuel systems. The fuel systems for diesel engines are complex, expensive systems that are critically important to meeting the efficiency and emissions targets of FCVT. Virtually every path to improving control of the combustion process in order to improve efficiency and lower emissions depends on improvements in the fuel injection system.

Fuel injectors are highly precise systems. The individual components must fit together with clearances sometimes smaller than 1×10^{-6} meters. Control of the combustion process requires precise control of the size, shape, and surface finish of the injector components.

The current systems for reliably controlling multiple injections are limited by the ability of mechanical and electronic systems to respond precisely and quickly enough to provide the additional control of injection. Smart materials, such as piezoelectric materials offer the potential of better control of fuel injection, and have been recently introduced for automobiles, but a number of improvements in the materials and manufacturing methods for the materials are yet required for heavy vehicles.

Presently, the fuel system represents a significant portion of the cost of a heavy-duty diesel engine. Enabling materials and cost-effective, precision manufacturing processes are instrumental in developing improved fuel injection systems. In addition to new and improved materials, improved manufacturing and inspection methods for the injector components are being developed as well.

Manufacturing technology for nickel aluminide - titanium carbide cermet fuel system components continued this year in coordinated efforts at ORNL, Southern Illinois University at Carbondale (SIUC), CoorsTek, Inc. and Cummins, Inc. ORNL prepared a large batch of processed powder which was provided to CoorsTek for injection molding of test components. The injection molded components were then sintered at ORNL and provided to Cummins for testing in fuel injection systems. In a parallel effort, SIUC evaluated a low-cost, high-throughput process, continuous belt sintering, for manufacturing the cermet components. SIUC determined that rapid heating, at rates up to 750°C/minute, resulted in higher densities and more uniform microstructures, and offer the potential for as much as 50% reduction in sintering costs by increasing part throughput.

Materials for exhaust aftertreatment. The reduction of NOx and particulate emissions is critically important to FCVT's program and is highly materials dependent. The DOE goals of improved efficiency of heavy vehicles are greatly complicated by engine design and exhaust aftertreatment technologies designed to meet the mandatory EPA emission regulations for 2007 and 2010. Materials and systems research is being conducted to minimize the potentially negative effects of emission-reduction technologies on fuel economy and to result in cleaner, more efficient engines.

Durability of exhaust aftertreatment systems in heavy vehicles is a concern. Lifetimes of at least 500,000 miles are expected, and 1,000,000 miles are desired (compared to 100,000 miles for automobiles). Exposure of the aftertreatment systems to high temperature, vibration, erosion, and chemical attack by species in the oil and fuel results in degradation of performance. Characterization of the effects of exposure in service on the microstructure and microchemistry of the aftertreatment systems is being conducted and may lead to development of more durable systems. The development of advanced NOx sensors is being conducted to facilitate optimal engine and aftertreatment control strategies.

Accomplishments this year include significant progress in a collaborative Ford–ORNL program whose objective is to facilitate deployment of NOx trap for lean diesel or gasoline exhaust by investigating materials issues related to deterioration of NOx trap performance upon aging as a result of thermal and sulfation-desulfation cycles, and investigating materials that are robust under the lean NOx trap operating conditions, including synthesis of new materials. Accomplishments include completion of the study of microstructural changes during aging under lean and rich conditions at 500°C of a series of model catalysts; beginning the updating of the ex-situ reactor to enable transmission electron microscopy samples under lean, rich, or stoichiometric conditions as well as lean-rich cycles; and equipping a new synthesis laboratory to enable preparation of NOx trap materials.

Research conducted at the High Temperature Materials Laboratory at ORNL is focused on the development and utilization of new capabilities and techniques for ultra-high resolution transmission electron microscopy (TEM) to characterize the microstructures of catalytic materials of interest for reduction of NOx emissions in diesel and automotive exhaust systems. This research aims to relate the effects of reaction conditions on the changes in morphology of heavy metal species on “real” catalyst support materials, typically oxides. Accomplishments include the characterization via high-resolution annular dark-field scanning transmission electron microscopy (STEM) imaging the structure of a model NOx trap material of near-atomic clusters and rafts of platinum atoms 1 to 3 atomic layers thick; characterization via TEM and STEM of core samples taken from catalyst monoliths removed from vehicles after up to 82,000 kilometers of driving; and taking delivery of the new aberration corrected electron microscope, which will enable imaging ultra-fine clusters of catalyst species on real catalyst samples of interest.

Cummins and ORNL collaborated, via CRADAs, in the characterization of laboratory- and engine-tested catalysts via X-ray diffraction, spectroscopy, and microscopy; and in the characterization of diesel particulate filters and the development of probabilistic design tools to predict the useful lifetime of the filters.

Ford Motor Company and ORNL are collaborating on the development of a NOx sensor that can be used in systems for on-board remediation of diesel engine exhausts. The sensor should have an operating temperature of 600–700^{o}C, and be able to measure NOx concentrations from 1 to 1500 ppm at oxygen levels from 5 to 20 vol. %. Prototype sensing elements are fabricated by patterning electronically conductive and catalytic layers onto oxygen-ion conducting substrates. The sensing elements are characterized for NOx response, oxygen sensitivity, and response time. Accomplishment this year include demonstrating NO2 sensing elements with extremely high sensitivity, demonstrating biased NO-selective sensing elements, and constructing both types of elements to consist of co-planar electrodes, one oxide electrode and the other a noble metal.

<u>Materials for air handling, hot section, and structural applications.</u> Engine design strategies for meeting EPA emission requirements have resulted in the need for significantly higher turbocharger boost. The higher boost requirements result in higher heat of compression and greater thermal and fatigue loads on turbocharger components.

Caterpillar and ORNL won a 2003 R&D 100 Award for the development of CF8C-Plus cast stainless steel. The new, high-temperature stainless steel may have near-term applications in diesel engine exhaust manifolds and turbocharger housings. Thermal-mechanical fatigue (TMF) of the initial commercial heats was completed this year, together with aging of various specimens. There was a significant advantage for CF8C-Plus relative to CN-12 or high SiMo cast iron in TMF testing to 760^{o}C. This year MetalTek International produced additional static sand-cast and centrifugally cast heats of CF8C-Plus for testing at Caterpillar and ORNL. That testing began this year and will be completed next year.

Caterpillar, in a collaboration with Argonne National Lab and ORNL, has a project to design and fabricate prototype engine valves from silicon nitride and titanium aluminide materials that are 30% lighter than steel valves, provide a 200% increase in service lifetime, and, potentially, a 10% increase in fuel efficiency in advanced engines. A probabilistic design approach was developed for the high-hardness valve materials. The friction welding of TiAl valve heads and Ti-6V-4Al valve stems was successfully optimized. The effects of surface finish on the performance of silicon nitride valves was evaluated and indicated that valves with good surface finish performed well in bench tests.

ORNL and Ricardo, Inc., evaluated the feasibility of reducing the weight of a heavy-duty engine by substituting a lighter material for the cast iron engine block and cylinder head. Finite element analysis was used to compute the stresses, temperatures, and fatigue safety factors of a 5.9L diesel engine, run at the maximum design power, for three lightweight casting alloy systems: a titanium alloy, aluminum alloy, and magnesium alloy. The analysis indicated feasibility of simple material substitutions in all cases, with the exception that the titanium alloy cylinder head will require inserts to reduce the temperature in the valve bridge area. Weight reduction of the entire engine by up to 33% for the magnesium alloy, 20% for the aluminum alloy; and uprating the power of the engine by 50% while reducing the weight by 15%, in the case of the titanium alloy, were predicted to be feasible.

Efforts in cost-effective manufacturing were carried out by ORNL, the University of Michigan, and Purdue University. Technology for machining difficult materials, such as titanium alloys, was developed in the ORNL/University of Michigan collaboration. ORNL investigated surface modification of lubricated ceramic parts for applications in fuel systems and related applications. Purdue University is investigating the consolidation of low-cost machining chips to produce nanocrystalline components with high strength and hardness.

In a new effort this year, ORNL is investigating the plastic deformation behavior of industrial ceramics and the potential for low-temperature forming of components. In collaboration with Pennsylvania State University, a novel sintering method was developed to fabricate nanocrystalline (less than 100 nm grain size) zirconia ceramics. Enhancement of plastic deformation of sub-micron zirconia in applied electric fields was observed in collaborative work with North Carolina State University. ORNL also established dynamic indentation and instrumented scratch testing facilities and associated finite element analysis models to characterize and model contact-induced damage and the links to wear performance and the optimization of machining and rolling contact fatigue.

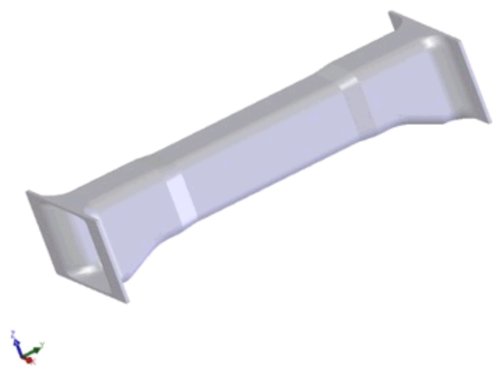
<u>Materials and testing standards.</u> FCVT has an International Energy Agency "Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications," (IA-AMT). The objectives of the IA-AMT are (1) to identify and evaluate promising new processing and surface engineering technologies capable of improving materials performance in transportation systems and (2) to promote and implement pre-competitive development and verification of advanced characterization methods appropriate for advanced materials for transportation applications. Annex III, which was approved in July 2002, consists of two subtasks on contact reliability of advanced engine materials including structural ceramics, composites, and nanostructured friction/wear coatings. Subtask 1 is an information exchange while Subtask 2 focuses on the development of standard test methods and procedures for the determination of rolling contact fatigue (RCF) resistance of advanced materials.

The RCF effort is led by ORNL. The objectives include the characterization of the RCF performance of ceramics and tribological coatings, determination of the effect of subsurface damage, microstructure, material properties, and contact stress on RCF performance, and correlation of RCF performance measured by different internationally used RCF test techniques. In this year a three-ball-on-rod test facility was established and informal collaboration was initiated with Bournemouth University in the United Kingdom.

High Strength Weight Reduction Materials

DOE's High-Strength Weight Reduction (HSWR) Materials Technology Development Area seeks to reduce parasitic energy losses due to the weight of heavy vehicles without reducing vehicle functionality, durability, reliability, or safety and to do so cost-effectively. The development area is focused on the development of materials and materials processing technologies that can contribute to weight reduction.

ORNL is collaborating with PNNL in an effort to overcome technical issues associated with joining composite materials in heavy vehicles. The project supports the industry-led effort to develop advanced composite support structures, including chassis lateral braces and primary beams for Class 7 and 8 vehicles. The initial focus of research is development and validation of one or more joint designs for a composite structural member attached to a metal member that together satisfy the truck chassis structural requirements both economically and reliably and with requisite durability.



Optimized geometry for lateral brace smoothed and drafted for manufacturability.

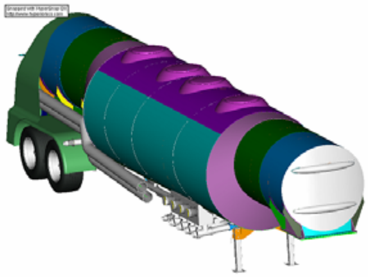
The multi-pronged approach includes evaluating a variety of hole fabrication techniques and their effects on subsequent performance; developing methods for detection of flaws and damage development during testing; static and fatigue testing under various environmental conditions; analyzing the effects of pre-load and bolt torque; and developing models for predicting the performance of joints. The results will be used to develop the first prototype composite component and joint for durability track testing in the latter part of 2005.

Magnesium alloys that have high specific strength (strength per unit of mass) are attractive materials for weight reduction. Presently, most magnesium use is limited to die-cast parts. Wrought magnesium alloys hold great promise for use in such components as hoods and doors. However, the need for a large number of processing steps and associated lengthy annealing times contributes to the high cost of sheet materials and presents one of the greatest barriers to the application of magnesium in these components.

Researchers at ORNL, in collaboration with industry and universities, are applying infrared processing technology to reduce this barrier. A successful demonstration run made at a commercial rolling mill equipped with a bank of infrared lamps produced materials with properties identical to those of materials produced with conventional techniques, but with much shorter annealing times and the potential for considerable cost savings. Future efforts will attempt to incorporate this technology with continuous twin roll casting to further reduce costs.

Infrared lamp rolling mill at Manufacturing Sciences, Inc., and close-up of magnesium alloy sheet exiting the roll gap.

As a result of a competitive solicitation, Heil Trailer International is working on a project to reduce the weight of an aluminum semi-trailer tanker by 20% through innovative design and the assimilation of composite materials into select components. ORNL is providing technical assistance and support to Heil. Excellent progress has been made on the vessel design and finite element analysis. Analysis, testing, and manufacturing studies have been completed successfully for the vessel and for the run gear/fifth wheel/bumper/underride. It is anticipated that the first full-scale prototype will be completed in 2005.

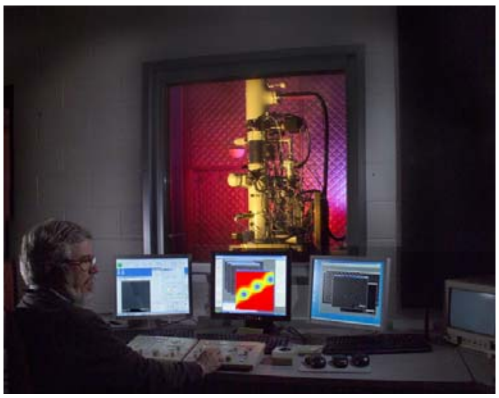


New concept petroleum trailer under development.

High Temperature Materials Laboratory

The High Temperature Materials Laboratory (HTML) User Program had an extremely successful year in FY 2004. A total of 87 new project proposals were received and reviewed, while activity on the 72 projects started last fiscal year continued. The new proposals were received from 28 industrial institutions, 54 colleges or universities, and 5 governmental agencies. Of the 87 proposals, 21 were from institutions that were new to the HTML this year. Most of the proposals came through the HTML User Program process, but a few represent collaborations with the Center for Nanophase Materials Science, an Office of Science, Basic Energy Sciences–sponsored activity at ORNL.

Fifty-three new User Agreements were negotiated by the Laboratory (5 university, 47 industry, and 1 other), which bodes well for continued growth of the User Program. More than a quarter (25) of the FY 2004 projects directly support the automotive industry, with interesting projects from Caterpillar, Ford Motor Company, Richard Childress Racing, and the General Motors R&D Center, among others. Seven of the proposals deal directly with hydrogen and fuel cells. Other projects support industrial processes, basic research, power generation, aerospace, and defense and homeland security.



Highlights of operations include the completion of the Advanced Microscopy Laboratory (AML), an ORNL General Purpose Projects–funded building adjacent to the HTML, designed to provide an extremely stable environment for electron microscopy. The Aberration-Corrected Electron Microscope (ACEM) was received and installation in AML was initiated. ACEM will be operational in FY2005. Also, a major upgrade was brought to completion on the Neutron Residual Stress Facility, a User Program–funded beamline at the High Flux Isotope Reactor at ORNL.

National Transportation Research Center

During FY 2004, the NTRC lost two key staff members. Richard E. Ziegler, director of the ORNL Transportation Program and manager of the NTRC User Facility, retired in February 2004. At about the same time, Dr. Steve Arnette, NTRC Director and University of Tennessee Condra Chair of Excellence in Automotive Systems, departed for personal reasons. Edmund T. Grostick, Deputy Director of the ORNL Transportation Program, has been filling Mr. Ziegler's positions in an acting capacity. A search is under way for a permanent replacement for Mr. Ziegler. Negotiations with the University of Tennessee to conduct a search for a replacement for Dr. Arnette are on-going.

Planning and negotiation continued on a facility co-located with the NTRC. This facility, called the Energy Conversion Research Facility (ECRF), would primarily provide additional analytical and engine test cell space for the Fuels, Engines, and Emissions Research Center; facilities for alternative liquid and gaseous fuels R&D; distributed energy powerplant R&D; and bench-scale analytic and experimental facilities for fuel cell R&D. The envisioned facility would be about 31,000 square feet, with just over half of that being dedicated research space, and the remainder for research support, storage, offices, and office support. Similar to the NTRC, the ECRF is planned to be built by a private third party and leased via long-term lease to ORNL. The facility could be ready for occupancy as early as FY 2007.

During FY 2004, eight external organizations inquired about establishing user agreements with the NTRC. Two of the inquiries were not suitable for user agreements. Six of the inquiries resulted in user projects. One project was performed in the Fuels, Engines and Emissions Research Center; two were performed in the Power Electronics and Electric Machinery Research Center; and three were performed in the composites laboratory on the Test Machine for Automotive Crashworthiness (TMAC). Increasing the number of users for the TMAC is an area of emphasis in FY 2005.

The ORNL Research Business Management Division has calculated the FY 2004 cost savings derived from housing researchers at the NTRC instead of on the main ORNL campus to be approximately $820,000, for a cumulative savings (FY 2002–2004) of approximately $2,796,400.

Vehicle Systems Analysis

FY 2004 saw limited activity in Vehicle Systems analytical efforts for FCVT as base funds were redirected to meet other DOE/FCVT obligations. In FY 2005, expectations are that increased activity will be realized in several prominent projects.

Within the Simulation and Validation portfolio of the program, ORNL actively participated in an Implementation Team charged with effecting the directives and recommendations of a comprehensive PSAT-Advisor assessment panel. Of particular note was the increased interaction with the ANL modeling efforts. ORNL provided data and supporting information to PSAT modelers at ANL (engine torque and speed maps over select operating regimes) for certain configurations of spark ignition engines applicable to hybrid powertrains being simulated at ANL. An aftertreatment sub-model for a diesel oxidation catalyst was provided as well.

In FY 2005, ORNL's modeling efforts in advanced engine concepts and aftertreatment schemes, developed for expected use in ADVISOR, will be reviewed and re-configured as needed for utilization in PSAT. In parallel, upgrades to the aftertreatment sub-models, which reflect recent developments, will be integrated. For example, the particle filter model will be upgraded to include aspects of particulate-characterizations conducted at Pacific Northwest National Laboratory. Alternately, exercises with advanced engine/combustion sub-models will be performed under the guidance of engine and vehicle systems tech teams by showing the performance requirements of the engine and its operating range in hybrid scenarios. The performance and fuel consumption maps of advanced virtual engines can then be imported into PSAT for vehicle-level calculations.

ORNL's development of the Automotive Systems Cost Model (ASCM) recommenced with some late year funds, and is being prepared for complementary interaction with the overall PSAT toolkit. As part of ORNL's participation in the implementation of DOE's

PSAT-oriented simulation strategy, we provided data to NREL on 13 EPA vehicle configurations for use in the Technical Targets Tool (T3) designed to estimate the effect of changing light-duty vehicle technical targets on the potential to reduce fuel use. Baseline cost estimates were developed for each of these vehicle configurations, both for today and for 2010. Distilled glider mass and cost relationships as a function of powertrain mass were also developed so that vehicle cost impacts due to a powertrain change could be considered in T3.

In the aforementioned activities, the ASCM will continue to be refined and integrated with the PSAT. Increased focus will be placed on the addition of operating and maintenance costs to achieve life-cycle cost approximations, and on introduction of fuel cell hybrids to the database. Markedly increased funding for this project in FY 2005 underscores the importance it brings to FCVT's decision support through independent cost analyses.

Within the Vehicle Systems Optimization portfolio, ORNL and DOE began the conclusion of a multi-year collaborative effort with NYSERDA and NYDOT in the completion of site selection, site design, truck hardware selection and the implementation of the selected designs for a shore power-based truck stop electrification (TSE) demonstration project. The ribbon cutting for the TSE facility occurred May 2004 in concurrence with the joint DOE/EPA National Idle Reduction Planning conference in Albany, New York. A dedicated fleet of 20 trucks was equipped with aftermarket shore power equipment that enables them to be plugged into stationary electric stanchions at the facility. Ending in FY 2005, this demonstration project will observe and address actual utilization of this available idle reduction technology, and altering the perceptions and behavior of targeted users.

A new modeling effort directed at aerodynamic drag reduction (at the wheel well of Class 8 line haulers) was commenced in late FY 2004, with the University of Tennessee-Chattanooga SimCenter. Dr. Whitfield of the SimCenter traveled to an Aerodynamic Drag Reduction consortium meeting held in Portland, Oregon, in July 2004. Arrangements were made at this meeting for the SimCenter to obtain specific geometries of interest, and to explore technology validation opportunities for fleet owners interested in testing drag reduction devices.

In addition, a new heavy-duty drive cycle task will commence in FY 2005. Using data logging equipment mounted on a small fleet of trailers, this task will produce actual use information on the duty cycle experienced by Class 8 heavy-duty trucks in a set of applications. One intention is to assist in identifying appropriate conditions for comparative evaluations with hybridized scenarios.